QCD on the lattice - an introduction
Lecture 3

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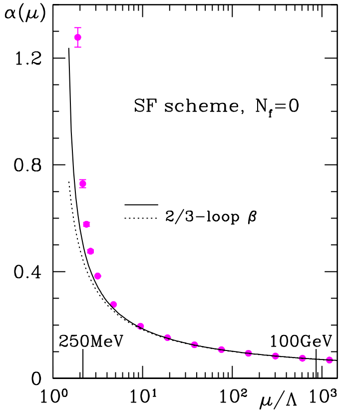
The running coupling

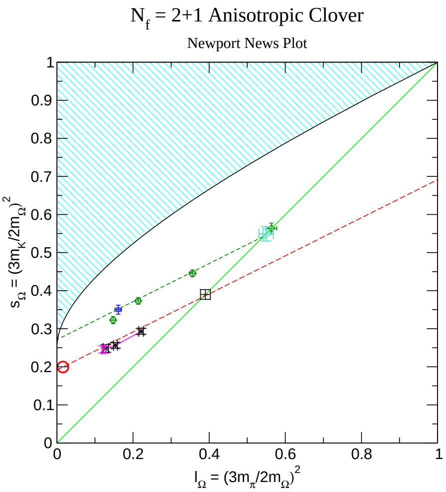
- The coupling in QCD effectively runs as a changes.
- QCD is **asymptotically free**, so as $a \to 0$, $\alpha_s(1/a) \to 0$.



- Run simulations with "bare" value of the coupling, β (and quark masses).
- Use one physical quantity to determine lattice spacing *post hoc*
- Use ratios of hadron masses to determine quark masses

from R. Sommer, `hep-ph/0607088`

Tuning quark masses



- To get to simulations of QCD with physical l, s quark masses requires tuning two more parameters m_l, m_s in the action.
- Work here at the lab (with Robert Edwards and Huey-Wen Lin)
- The physical point is currently inaccessible - too expensive to run simulations there.

QCD on the computer - Monte Carlo integration

- On a finite lattice, with non-zero lattice spacing, the number of degrees of freedom is finite. The path integral becomes an "ordinary" high-dimensional integral.
- High-dimensional integrals can be estimated stochastically by Monte Carlo. Variance reduction is crucial, and can be achieved effectively provided the theory is simulated in the Euclidean space-time metric.
- No useful importance sampling weight can be written for the theory in Minkowski space.
- The Euclidean path-integral is a weighted average:

$$\langle \mathcal{O} \rangle = \frac{1}{Z} \int \mathcal{D}U \mathcal{D}\bar{\psi} \mathcal{D}\psi \;\; \mathcal{O}[U, \bar{\psi}, \psi] \, e^{-S[U,\bar{\psi},\psi]}$$

- e^{-S} varies enormously; sample only the tiny region of configuration space that contributes significantly.

Importance sampling

- **Importance sampling** is a **variance reduction** method.
- Variance reduction: we can construct stochastic estimates of the integral of interest that have lower variances. This means the standard error for a given sample size is lower.
- This is extremely effective for many high-dimensional integrals that arise in theoretical physics (statistical physics, thermodynamics, field theory, . . .).
- The fraction of phase space that contribute significantly is miniscule - we want methods to generate points only in these important regions $=$ importance sampling.

Importance sampling

- Consider the D dimensional integral,

$$I = \int_V f(x) \; d^D x = \int_V \frac{f(x)}{g(x)} \; g(x) dx$$

- Generate points $\{x_1, x_2, x_3, \dots\}$ in V with probability density $g(x)$.
- Then for $i = 1 \dots n$, compute $h_i = \frac{f(x_i)}{g(x_i)}$ over the sample points. The theory of Monte Carlo gives

$$E(h) = \int_V h(x) g(x) dx = I$$

- The expected value of h is the integral, I so averaging h_i gives an unbiased estimate of I.

Importance sampling

- So how has changing the sampling probability helped?
- The uncertainty in our estimator is related to its variance.

$$\mathrm{var}(h) = E(h^2) - E(h)^2$$

and

$$E(h^2) = \int \frac{f^2(x)}{g^2(x)}\; g(x)dx = \int \frac{f^2(x)}{g(x)} dx$$

- The expected value of h is I, and so independent of g but the variance of the estimator does depend on h.
- The optimal choice for h is

$$h_{\rm opt}(x) = \frac{|f(x)|}{\int_V |f(x)| dx}$$

- It is usually impractical to find $h_{\rm opt}$, but this result hints how to improve the sampling - sample regions where f is large more often.

Benefits of importance sampling

- Examples of the benefits of importance sampling

$$I_0(z) = \int_0^z e^{-x} sin^2 \pi x^2 \;\; dx$$

Flat Sampling - 10,000,000 samples

z	MC estimator $\pm$ error
1.0	0.197192 ± 0.000058
10.0	0.37907 ± 0.00029
100.0	0.37818 ± 0.00097
1000.0	0.3768 ± 0.0031

Importance sampling $p(x) \propto e^{-x}$ 10,000,000 samples

z	MC estimator $\pm$ error
1.0	0.197115 ± 0.000070
10.0	0.37902 ± 0.00011
100.0	0.37895 ± 0.00011
1000.0	0.37908 ± 0.00011

Dynamical quarks in QCD

- Monte Carlo integration with $N_f = 2$ (mass degenerate) quarks. Quark fields in the path integral obey a grassmann algebra which is difficult to manipulate in the computer.
- The quark action is a bilinear; the grassmann integrals can be done analytically and give

$$Z_Q[U] = \int \mathcal{D}\psi \mathcal{D}\bar{\psi} \;\; e^{-\sum_f \bar{\psi}_f M[U]\psi} = \det M^{N_f}[U]$$

- The full partition function, including the gauge fields is

$$Z = \int \mathcal{D}U \;\; Z_Q[U] e^{-S_G[U]} = \int \mathcal{D}U \;\; \det M^{N_f}[U] e^{-S_G[U]}$$

- For (eg) $N_f = 2 \det M^2$ is positive and can be included in the importance sampling. It is a non-local function of the gauge fields, and expensive to compute. Using $M^\dagger = \gamma_5 M \gamma_5$, $\det M^2$ is re-written

$$Z_Q[U] = \int \mathcal{D}\phi \mathcal{D}\phi^* e^{-\phi^* [M^\dagger M]^{-1} \phi}$$

Dynamical quarks in QCD

- ϕ is an unphysical (non-local action) bosonic field with colour charge and spin structure (!) called the pseudofermion.
- Measuring the action requires applying the inverse of M a very large matrix
- M is sparse, and there are a set of linear algebra tricks (Krylov space solvers etc) that work effectively.
- Unfortunately, they require many applications of the matrix to a quark field, and so take a lot of computer time.
- This is where most computing power in lattice simulations goes; computing the effect of the quark fields acting on the gluons in the Monte Carlo updates.
- The alternative is the quenched approximation to QCD; ignore the fermion path integral completely - this is an unphysical approximation so its effects are hard to quantify.
- Inversion is needed again in the measurement stage too;

$$\langle\psi(x)\bar{\psi}(y)\rangle = M^{-1}[U](x,y)$$

Markov Chain Monte Carlo

- How is the configuration space sampled?
- All techniques use a **Markov process**: this is a stochastic transition that takes the current state of the system and jumps randomly to a new state, such that the probability of the jump is independent of the past states of the system.
- Ergodic (positive recurrent, irreducible) Markov chains have unique stationary distributions; build the Markov process so it has our importance sampling distribution as its stationary state.
- If this can be done, then the sequence of configurations generated by the process is our importance sampling ensemble!
- Almost all algorithms exploit **detailed balance** to achieve this.

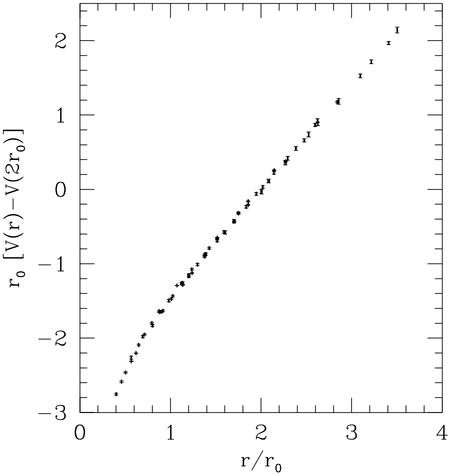
Some physics: the confining string (2)

- Now for some physics!
- One of the first physical quantities calculated on the lattice is the (confining) potential energy of two static colour sources, separated by distance R
- Energies are measured by examining the fall-off of a two-point correlation function measured in the path integral by Monte Carlo.
- What would appropriate gauge invariant operators look like for the static potential?

$$a^\dagger(R,t) = \sum_{\underline{x}} \bar{Q}(\underline{x},t) U_i(\underline{x},t) U_i(\underline{x}+\hat{\imath}) \ldots U_i(\underline{x}+(R-1)\hat{\imath}) Q(\underline{x}+R\hat{\imath},t)$$

- If the mass of the field Q is taken very large, the propagator becomes proportional to just a time-like string of gauge fields
- So the potential can be measured by computing the expectation value of large, flat space-time loops of gauge fields.

The confining string (2)



from C. Morningstar and M.P, Phys.Rev.D56:4043-4061,1997 `hep-lat/9704011`

Summary

- Lattice bare couplings determine the lattice spacing and meson spectrum, so making contact with physics implies β is a function of a (they are not independent).
- The best way of tuning bare quark masses is still a research topic. In principle there are lots of perfectly fine definitions.
- Making non-perturbative predictions from the lattice QCD path integral requires numerical attack - **Monte Carlo simulations**
- The quarks present a particular challenge - the grassmann integrals are difficult to manipulate directly
- They can however be integrated out analytically, leaving a non-local action on the gauge fields.
- Manipulating the dynamics of this action requires evaluation of the inverse of a large, sparse matrix - this is the **computationally expensive** part of lattice calculations.